

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 2.09e-02 mol/L

Global applicability domain: Inside

Local applicability domain index: 7.72e-01

Confidence level: 7.10e-01

Nearest Neighbors from the Training Set

Image not found

Bromoethane

Measured: 8.20e-02

Predicted: 4.02e-02

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1-Propene

Measured: 4.75e-03

Predicted: 6.81e-03

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Ethylene

Measured: 4.67e-03

Predicted: 7.89e-03

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Methyl bromide

Measured: 1.60e-01

Predicted: 9.95e-02

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1,3-Butadiene

Measured: 1.36e-02

Predicted: 1.80e-02